

chain nodes :  
 12 13 14 15 16 17  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 10 11  
 chain bonds :  
 5-7 12-13 14-16 16-17  
 ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11  
 exact/norm bonds :  
 7-8 7-11 8-9 9-10 10-11 12-13 14-16 16-17  
 exact bonds :  
 5-7  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6

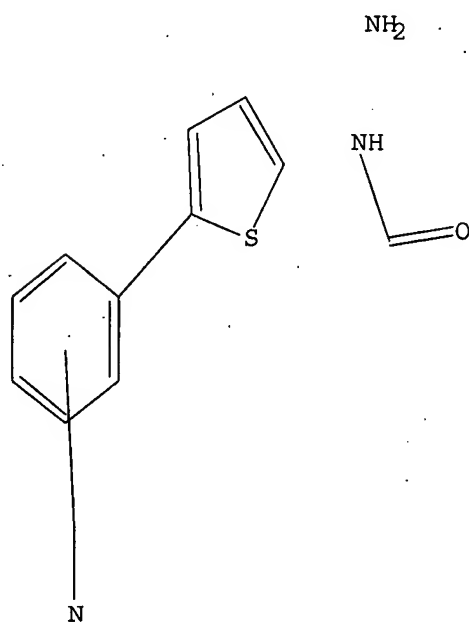
Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom

L3 STRUCTURE UPLOADED

=> d

L3 HAS NO ANSWERS

L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l3 full

FULL SEARCH INITIATED 14:30:51 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 225853 TO ITERATE

100.0% PROCESSED 225853 ITERATIONS

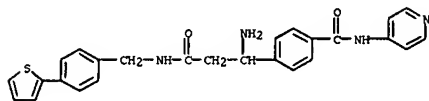
SEARCH TIME: 00.00.01

182 ANSWERS

L4 182 SEA SSS FUL L3

=> d l4 -10

L4 ANSWER 1 OF 182 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 920497-15-0 REGISTRY  
 ED Entered STN: 12 Feb 2007  
 CN Benzenepropanamide,  $\beta$ -amino-4-[(4-pyridinylamino)carbonyl]-N-[(4-(2-thienyl)phenyl)methyl]- (CA INDEX NAME)  
 MF C26 H24 N4 O2 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

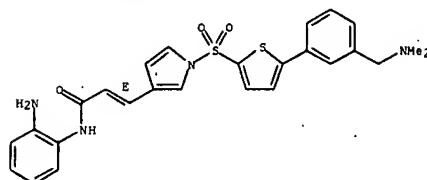


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 2 OF 182 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 910463-22-8 REGISTRY  
 ED Entered STN: 16 Oct 2006  
 CN 2-Propenamide, N-(2-aminophenyl)-3-[1-[(5-[3-[(dimethylamino)methyl]phenyl]-2-thienyl)sulfonyl]-1H-pyrrol-3-yl]-, (2E)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C26 H26 N4 O3 S2  
 CI COM  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

Double bond geometry as shown.

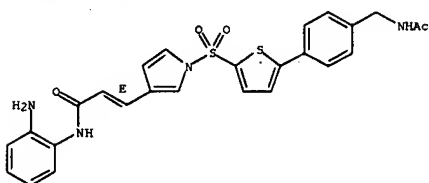


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 3 OF 182 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 910463-21-7 REGISTRY  
 ED Entered STN: 16 Oct 2006  
 CN 2-Propenamide, 3-[1-[(5-[4-[(acetylamino)methyl]phenyl]-2-thienyl)sulfonyl]-1H-pyrrol-3-yl]-N-(2-aminophenyl)-, (2E)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C26 H24 N4 O4 S2  
 CI COM  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

Double bond geometry as shown.

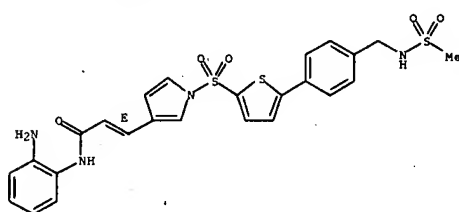


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 4 OF 182 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 910463-19-3 REGISTRY  
 ED Entered STN: 16 Oct 2006  
 CN 2-Propenamide, N-(2-aminophenyl)-3-[1-[(5-[4-[(methylsulfonyl)amino]methyl]phenyl)-2-thienyl)sulfonyl]-1H-pyrrol-3-yl]-, (2E)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C25 H24 N4 O5 S3  
 CI COM  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

Double bond geometry as shown.

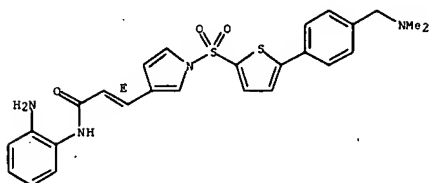


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 5 OF 182 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 910463-04-6 REGISTRY  
 ED Entered STN: 16 Oct 2006  
 CN 2-Propenamide, N-(2-aminophenyl)-3-[[[5-[4-[(dimethylamino)methyl]phenyl]-2-thienyl]sulfonyl]-1H-pyrrol-3-yl]-, (2E)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C26 H26 N4 O3 S2  
 CI COM  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

Double bond geometry as shown.

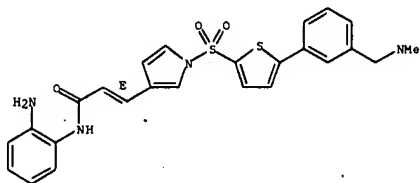


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 6 OF 182 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 910461-18-6 REGISTRY  
 ED Entered STN: 16 Oct 2006  
 CN 2-Propenamide, N-(2-aminophenyl)-3-[[[5-[3-[(dimethylamino)methyl]phenyl]-2-thienyl]sulfonyl]-1H-pyrrol-3-yl]-, hydrochloride, (2E)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C26 H26 N4 O3 S2 . x Cl H  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER  
 CRN (910463-22-8)

Double bond geometry as shown.

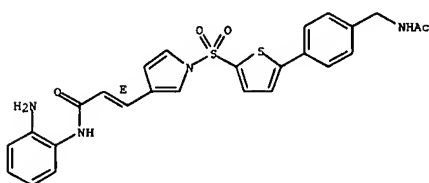


● x HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 7 OF 182 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 910461-17-5 REGISTRY  
 ED Entered STN: 16 Oct 2006  
 CN 2-Propenamide, 3-[[[5-[4-[(acetylamino)methyl]phenyl]-2-thienyl]sulfonyl]-1H-pyrrol-3-yl]-N-(2-aminophenyl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C26 H24 N4 O4 S2 . Cl H  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER  
 CRN (910463-21-7)

Double bond geometry as shown.

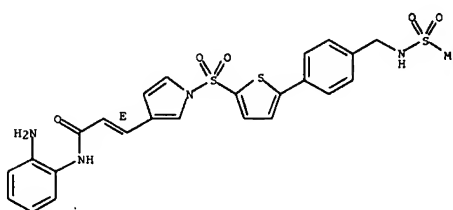


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 8 OF 182 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 910461-15-3 REGISTRY  
 ED Entered STN: 16 Oct 2006  
 CN 2-Propenamide, N-(2-aminophenyl)-3-[[[5-[4-[(methylsulfonyl)amino]methyl]phenyl]-2-thienyl]sulfonyl]-1H-pyrrol-3-yl]-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C25 H24 N4 O5 S3 . Cl H  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER  
 CRN (910463-19-3)

Double bond geometry as shown.

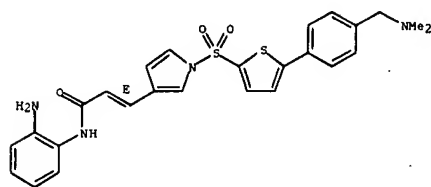


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 9 OF 182 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 910460-98-9 REGISTRY  
 ED Entered STN: 16 Oct 2006  
 CN 2-Propenamide, N-(2-aminophenyl)-3-[[1-[[5-[[4-[[dimethylamino)methyl]phenyl]-2-thienyl]sulfonyl]-1H-pyrrol-3-yl]-, hydrochloride, (2E)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C26 H26 N4 O3 S2 . x C1 H  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER  
 CRN (910463-04-6)

Double bond geometry as shown.

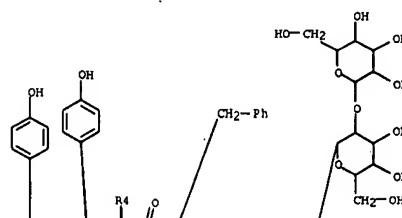


• x HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

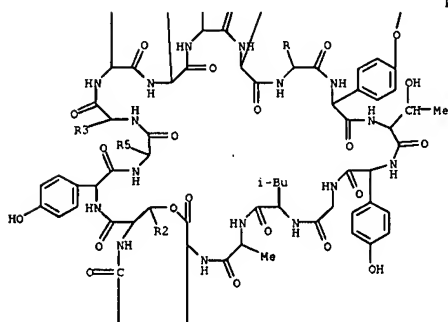
L4 ANSWER 10 OF 182 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 910318-81-9 REGISTRY  
 ED Entered STN: 13 Oct 2006  
 CN Ramoplanin A 1, 1-[N2-[4-(2-thienyl)benzoyl]-L-asparagine]- (9CI) (CA INDEX NAME)  
 FS PROTEIN SEQUENCE/ STEREOSEARCH  
 MF C121 H148 C1 N21 O40 S  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 \*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

PAGE 1-A

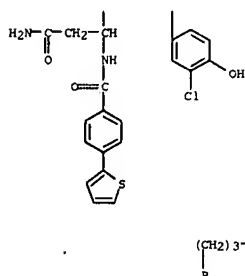


L4 ANSWER 10 OF 182 REGISTRY COPYRIGHT 2007 ACS on STN (Continued)

PAGE 2-A

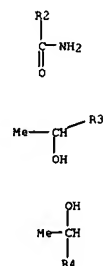


PAGE 3-A

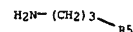


L4 ANSWER 10 OF 182 REGISTRY COPYRIGHT 2007 ACS on STN (Continued)

PAGE 4-A

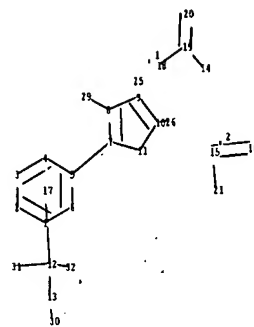
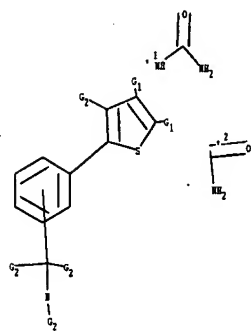


PAGE 5-A



1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=>  
Uploading C:\Program Files\Stnexp\Queries\10542326g.str



chain nodes :

L5        STRUCTURE UPLOADED

=> d

L5 HAS NO ANSWERS

L5                STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l5 fulk

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID

The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=> s l5 ful

FULL SEARCH INITIATED 14:39:28 FILE 'REGISTRY'

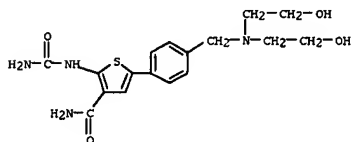
FULL SCREEN SEARCH COMPLETED -        1051 TO ITERATE

100.0% PROCESSED        1051 ITERATIONS  
SEARCH TIME: 00.00.01

64 ANSWERS

L6                64 SEA SSS FUL L5

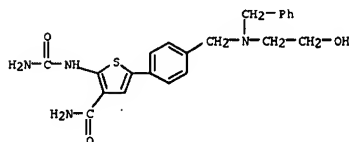
L6 ANSWER 1 OF 64 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 728948-24-1 REGISTRY  
 ED Entered STN: 19 Aug 2004  
 CN 3-Thiophenecarboxamide, 2-[(aminocarbonyl)amino]-5-[4-[[bis(2-hydroxyethyl)amino)methyl]phenyl]- (9CI) (CA INDEX NAME)  
 MF C17 H22 N4 O4 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

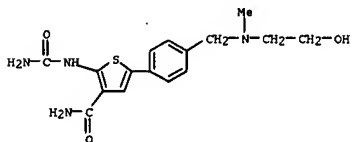
L6 ANSWER 2 OF 64 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 728948-23-0 REGISTRY  
 ED Entered STN: 19 Aug 2004  
 CN 3-Thiophenecarboxamide, 2-[(aminocarbonyl)amino]-5-[4-[[[(2-hydroxyethyl)(phenylmethyl)amino)methyl]phenyl]- (9CI) (CA INDEX NAME)  
 MF C22 H24 N4 O3 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

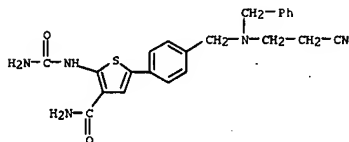
L6 ANSWER 3 OF 64 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 728948-22-9 REGISTRY  
 ED Entered STN: 19 Aug 2004  
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 MF C16 H20 N4 O3 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 4 OF 64 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 728948-21-8 REGISTRY  
 ED Entered STN: 19 Aug 2004  
 CN 3-Thiophenecarboxamide, 2-[(aminocarbonyl)amino]-5-[4-[[[(2-cyanoethyl)(phenylmethyl)amino)methyl]phenyl]- (9CI) (CA INDEX NAME)  
 MF C23 H23 N5 O2 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

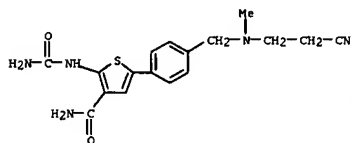


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)



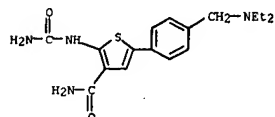
L6 ANSWER 5 OF 64 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 728948-20-7 REGISTRY  
 ED Entered STN: 19 Aug 2004  
 CN 3-Thiophenecarboxamide, 2-[(aminocarbonyl)amino]-5-[4-[(2-cyanoethyl)methylamino]methyl]phenyl]- (9CI) (CA INDEX NAME)  
 MF C17 H19 N5 O2 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

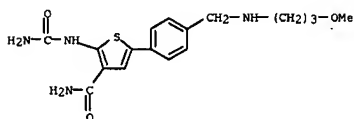
L6 ANSWER 6 OF 64 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 728948-19-4 REGISTRY  
 ED Entered STN: 19 Aug 2004  
 CN 3-Thiophenecarboxamide, 2-[(aminocarbonyl)amino]-5-[4-[(diethylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)  
 MF C17 H22 N4 O2 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

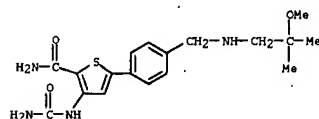
L6 ANSWER 7 OF 64 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 728948-18-3 REGISTRY  
 ED Entered STN: 19 Aug 2004  
 CN 3-Thiophenecarboxamide, 2-[(aminocarbonyl)amino]-5-[4-[(3-methoxypropyl)amino]methyl]phenyl]- (9CI) (CA INDEX NAME)  
 MF C17 H22 N4 O3 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

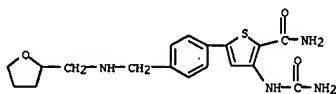
L6 ANSWER 8 OF 64 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 728948-17-2 REGISTRY  
 ED Entered STN: 19 Aug 2004  
 CN 2-Thiophenecarboxamide, 3-[(aminocarbonyl)amino]-5-[4-[(2-methoxy-2-methylpropyl)amino]methyl]phenyl]- (9CI) (CA INDEX NAME)  
 MF C18 H24 N4 O3 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

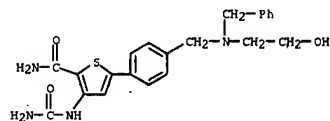
L6 ANSWER 9 OF 64 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 728948-16-1 REGISTRY  
 ED Entered STN: 19 Aug 2004  
 CN 2-Thiophenecarboxamide, 3-[(aminocarbonyl)amino]-5-[4-[[[(2-tetrahydro-2-furanyl)methyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)  
 MF C18 H22 N4 O3 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 10 OF 64 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 728948-15-0 REGISTRY  
 ED Entered STN: 19 Aug 2004  
 CN 2-Thiophenecarboxamide, 3-[(aminocarbonyl)amino]-5-[4-[[[(2-hydroxyethyl)(phenylmethyl)amino]methyl]phenyl]- (9CI) (CA INDEX NAME)  
 MF C22 H24 N4 O3 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
564.30	564.51

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 14:40:49 ON 04 AUG 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907 - 4 Aug 2007 VOL 147 ISS 7  
FILE LAST UPDATED: 3 Aug 2007 (20070803/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l6  
L7 1 L6

=> d l7 ibib abs

L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:606462 CAPLUS

DOCUMENT NUMBER: 141:157027

TITLE: Preparation of thiophenylcarboxamides as IKK-2 inhibitors for the treatment of inflammatory diseases.

INVENTOR(S): Faull, Alan Wellington; Johnstone, Craig; Morley, Andrew David; Poyser, Jeffrey Philip

PATENT ASSIGNEE(S): AstraZeneca Ab, Swed.; AstraZeneca UK Limited

SOURCE: PCT Int. Appl., 59 pp.

DOCUMENT TYPE: Patent

LANGUAGE: English

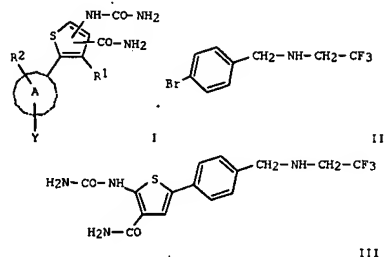
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004063186	A1	20040729	WO 2004-GB96	20040113
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, GU, HK, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LX, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ				
EP 1583755	A1	20051012	EP 2004-701627	20040113
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006516273	T	20060629	JP 2006-500200	20040113
US 2006058522	A1	20060316	US 2005-542326	20050713
PRIORITY APPLN. INFO.: SE 2003-92 A 20030115				
OTHER SOURCE(S): MARPAT 141:157027 W 20040113				
GI				

L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

bromide II, e.g., prepd. from 4-bromobenzylbromide and 2,2,2-trifluoroethylamine, afforded thiophenylcarboxamide III. In IKK-2 filter kinase inhibition assays, 4-examples of compds. I exhibited IC50 values ranging from 0.00056-0.066  $\mu$ M, e.g., the IC50 value of thiophenylcarboxamide III was 0.0036  $\mu$ M. Compds. I are claimed useful for the treatment of inflammatory diseases.



AB Title compds. I [R1 = H, CH3; R2 = H, halo, CN, etc.; R3, R4 = H, CH3; A = 6-membered aromatic ring optionally incorporating one or two nitrogen atoms; X = NR6; R5 = H, Cl, alkyl, etc.; R6 = H, Cl, alkyl] and their pharmaceutically acceptable salts were prepared For example, Pd mediated coupling of 2-[(aminocarbonyl)amino]-5-bromothiophene-3-carboxamide and